# ABSTRACT

The distribution of chemical compounds in high-dimensional molecular descriptor space can be viewed in two dimensions by applying the projection method of this invention. This method has particular usefulness for viewing the relationships of a large number of compounds such as found in a large scale HTS or virtual combinatorial library. After selecting a representative subset of the larger data set of compounds, initially components from the high-dimensional descriptor space are determined by PCA. In order to relax an NLM projection using the PCA components as a start, the stress function is modified to reflect a local horizon beyound which the separation of the compounds is not meaningfully measureable. The resulting two dimensional projections provide a clear insight into the distribution of the chemical compounds in the higher dimensional space. The method is clearly generalizable to viewing descriptor space in three dimensions and to using high dimensional descriptors other than those used to describe molecular structure.